

From: [HOPE Bruce](#)
To: [Eric Blischke/R10/USEPA/US@EPA](#)
Subject: RE: Relationship of Kow and Koc
Date: 12/18/2007 07:23 AM

Eric,
Mackay (2001) reports a study of 170 correlations between KOW & KOC. These 170 correlations suggest that KOC is best approximated as $0.35 \times \text{KOW}$. This is not far from the $0.41 \times \text{KOW}$ also reported in Mackay (2001) and attributed to Karickhoff (1981). Karickhoff et al.'s 0.63 value might be based on only a subset of chemicals. No single correlation has been shown to be applicable to all substances and these correlation factors can vary by a factor of 2.5. Thus, depending on the nature of the organic carbon, KOC can be as high as $0.90 \times \text{KOW}$ and as low as $0.14 \times \text{KOW}$. I use 0.41 to conform to Mackay (who suggests that either 0.35 or 0.41 would be OK), except when calculating the bioavailable solute fraction, where 0.35 is used to conform to the work of Gobas on uptake in aquatic systems.
Bruce

-----Original Message-----

From: Blischke.Eric@epamail.epa.gov
[mailto:Blischke.Eric@epamail.epa.gov]
Sent: Monday, December 17, 2007 5:12 PM
To: HOPE Bruce
Subject: Relationship of Kow and Koc

Bruce, I wanted to perform some quick and dirty sediment to porewater partitioning analyses. The information presented in the Round 2 Report and Fate and Transport Model Report focus on Kow and not Koc. However, it appears that you developed a "Constant for OC partition coefficient from Kow" - Cnkoc - with an estimated value of 0.35. I also found this tidbit on the internet:

Karickhoff, et al. developed an empirical relationship between Koc and Kow. They studied the sorption of hydrophobic organic compounds on pond and river sediments and found that there was a linear relationship between Koc (for sediment particles < 50 um) and Kow:

$$\text{Koc} = 0.63 \text{ Kow} \quad (r^2 = .96)$$

Of course the two approaches don't exactly match up. Typically, I consult my GW Chemical Desk Reference for literature Koc's but wanted to be consistent with information presented in project documents. Any advice on a simple way to go?

Thanks, Eric